

Numerical Simulation of Lean Premixed Turbulent Hydrogen/Hydrocarbon Flames at Elevated Pressures

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Outline

- ⌄ Kobayashi data
- ⌄ A relatively novel reaction model
- ⌄ Model predictions – ,blended‘ fuels – Two flame data
- ⌄ A submodel for the critical chemical time scale

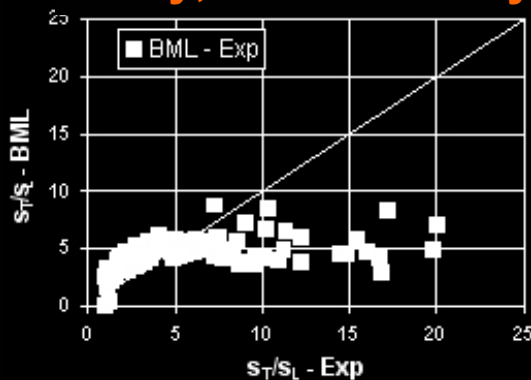
(H₂-doped) Hydrocarbon Lean Flames

- ⚡ Hydrocarbon Combustion at Lean flammability limit yields low NO_x**
- ⚡ Low operating temperatures cause low flame speeds and are susceptible to flame instability**
- ⚡ Hydrogen enrichment substantially improves the flame speed and extinction characteristics**

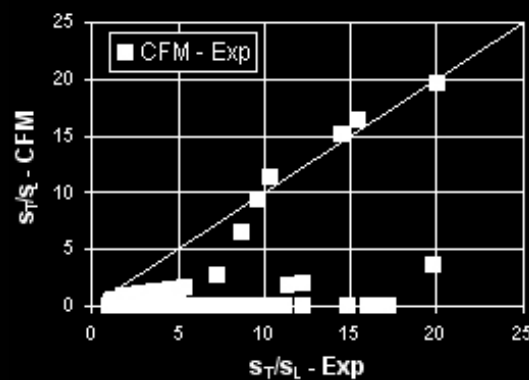
Pressure & Fuel Influence – Different Models

Flame Angle (dimensionless): Computed vs. Measured

Bray, Moss & Libby



Marble and Broadwell



Kobayashi Data

$\text{CH}_4, \text{C}_2\text{H}_4, \text{C}_3\text{H}_8$

$\text{Re}_t \leq 1340$

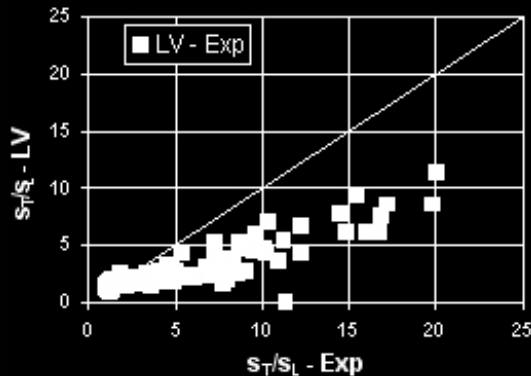
$u'/S_L \leq 25$

$\phi = 0.5, 0.7, 0.9$

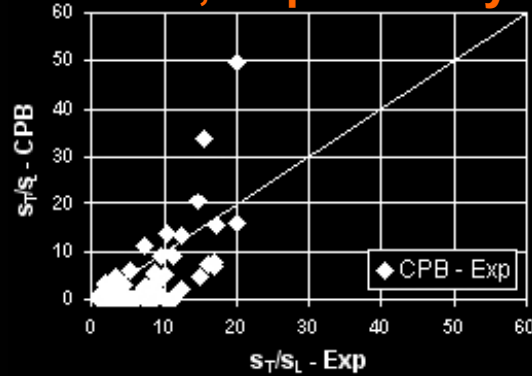
$p = 1, 5, 10, 20, 30 \text{ bar}$

$Le = 1.0, 1.2, 1.6$

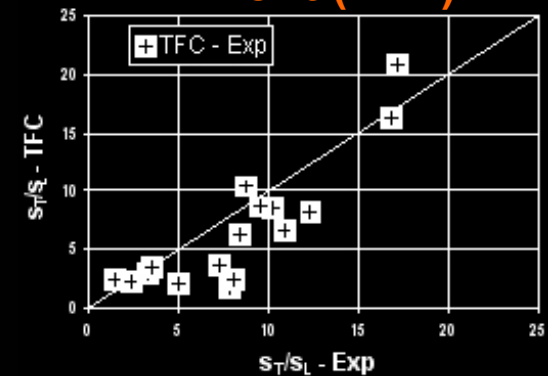
Lindstedt and Váos



Cant, Pope & Bray



Zimont (TFC)



Algebraic Flame Surface Wrinkling Model

General reaction rate expression $\bar{w}_c = \rho_u s_L I_0 \Sigma$

Damköhler's hypothesis

$$\frac{A_T}{\bar{A}} \sim \frac{s_T}{s_L}$$

$$\bar{w}_{turb.} = w_{lam.} \cdot \Sigma$$

Reaction locally similar to laminar

$$w_{lam.} = \rho_u \cdot s_L$$

Folding factor Σ = Flame surface area / Volume

$$\Sigma = \frac{A_T}{\bar{A}} \cdot |\nabla \tilde{c}|$$

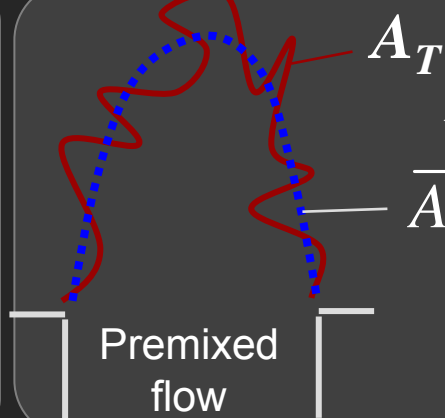
Surface density function

$$= \left\{ \sum_{j=1}^3 \left(\frac{\partial \tilde{c}}{\partial x_j} \right)^2 \right\}^{1/2}$$

A_T
Turbulent flame surface area

\bar{A}
Projected flame surface area

Premixed turbulent flame



$$\frac{A_T}{\bar{A}} = f(\text{Re}_t, u', p, \dots)$$

That is, all the statistical properties of turbulent premixed flames are universally and unambiguously controlled by: the length scale, mean dissipation rate, viscosity and chemical time scale

Novel Submodel for Turbulent Flame Speed

$$S_T = S_{L0} \left(1 + \frac{A}{\exp(Le - 1)} \text{Re}_t^{0.25} \left(\frac{u'}{S_{L0}} \right)^{0.3} \left(\frac{p}{p_0} \right)^{0.2} \right)$$

in time scales

$$S_T = S_{L0} + \frac{A}{\exp(Le - 1)} \left(u'^{0.8} S_{L0}^{0.2} \right) (Da)^{1/4} \left(\frac{p}{p_0} \right)^{0.2}$$

↓

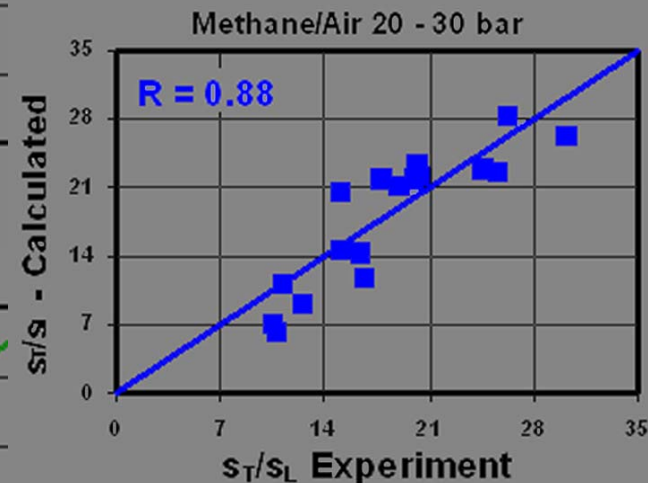
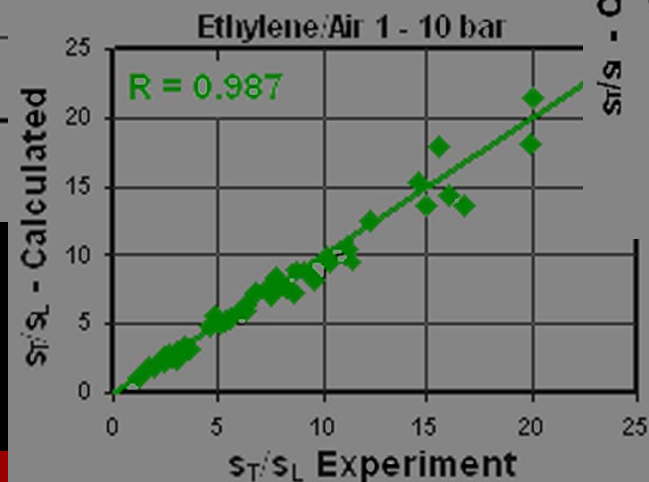
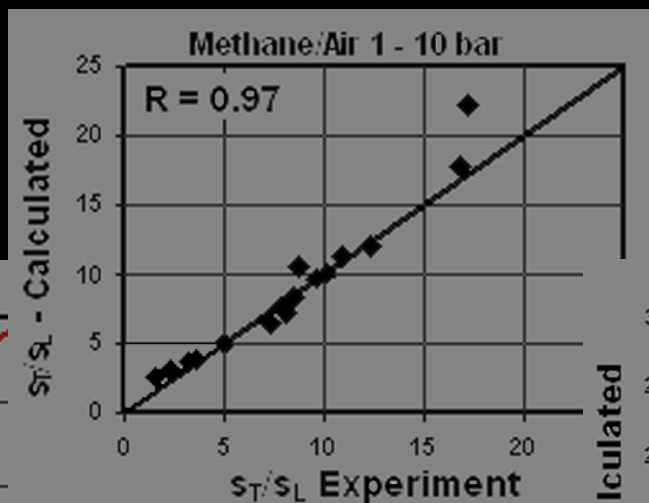
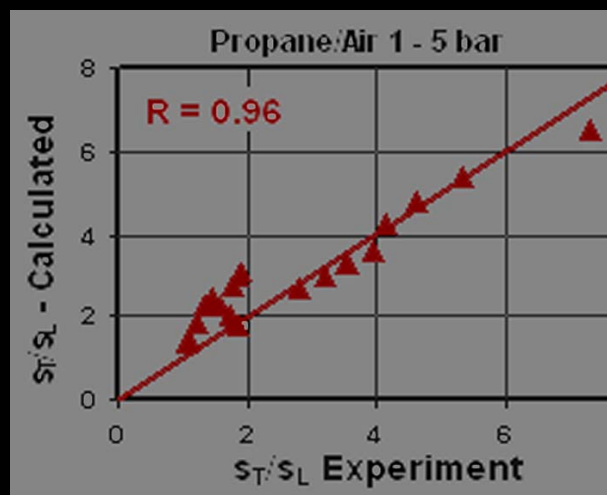
$$\text{Damköhler number } Da = \frac{\tau_t}{\tau_c} = \frac{l_x / u'}{\delta_{L0} / S_{L0}}$$

Novel Submodel - in older form

$$S_T = S_{L0} \left(1 + \frac{A}{Le} \text{Re}_t^{0.25} \left(\frac{u'}{S_{L0}} \right)^{0.3} \left(\frac{p}{p_0} \right)^{0.2} \right)$$

Turbulent flame speed proportional to $1/Le$ is similar to one of the Bradley's ST relations (shown by Driscoll in yesterday's presentation), but has been independantly obtained

Correlation plots – All hundred+ data



Rxn Closure extrapolated
for 20 and 30 bar

Five different flames

Hydrocarbons (HC)

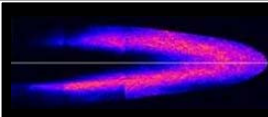
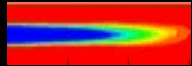
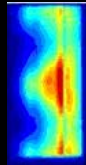
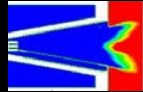
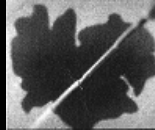
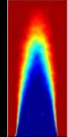
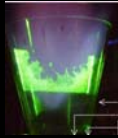
1. High-jet enveloped flame
2. GT burner-combustor flame

Hydrogen and Hydrocarbons

3. Expanding spherical flame

HC & Hydrogen-doped HC flames

4. Bunsen-like flame
5. Novel Wide-angled Diffuser flame

Exp	Num	
		Done (14 bar)
		Done (32 bar) Le <= 2.3
		Analytical evaluation
		In progress (9 bar)
		Planned

1. Griebel et al., (Switzerland)
2. ALSTOM (Switzerland)

3. Kido et al., (Japan)
4. Gökalp et al. (France)

5. Lawn (UK)

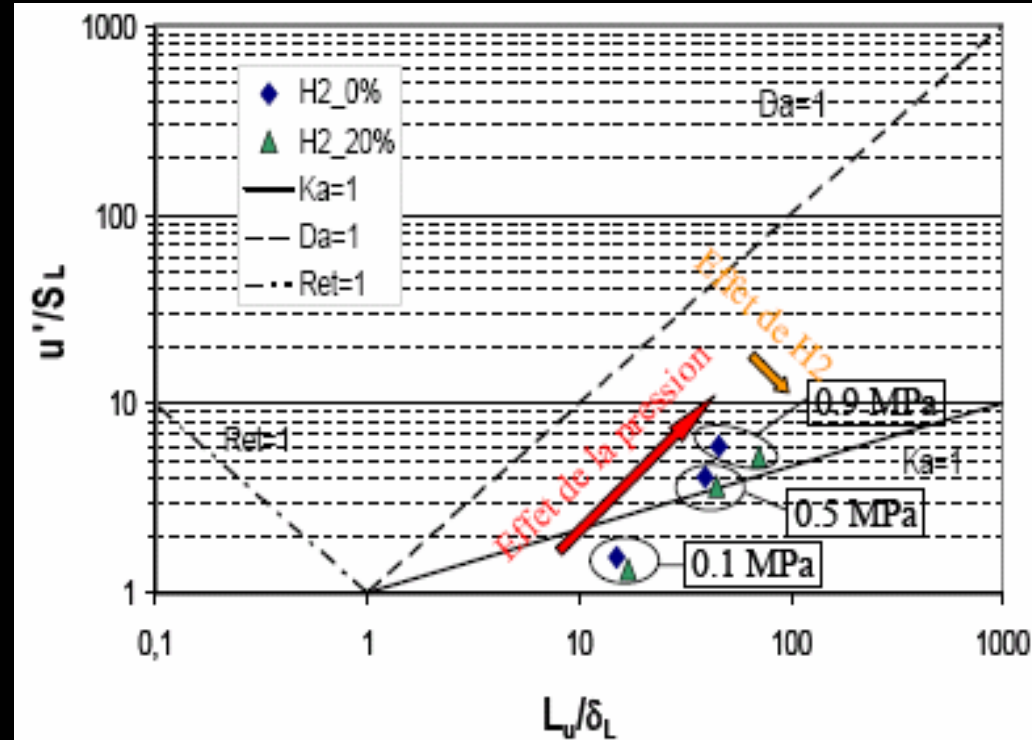
H₂-doped Premixed Turbulent Flames – Halter et al.

Nine lean ($\phi=0.6$) CH₄ **Bunsen** flames

Pressure 1, 5, 9 bar; $u'/S_{L0} \leq 5.5$

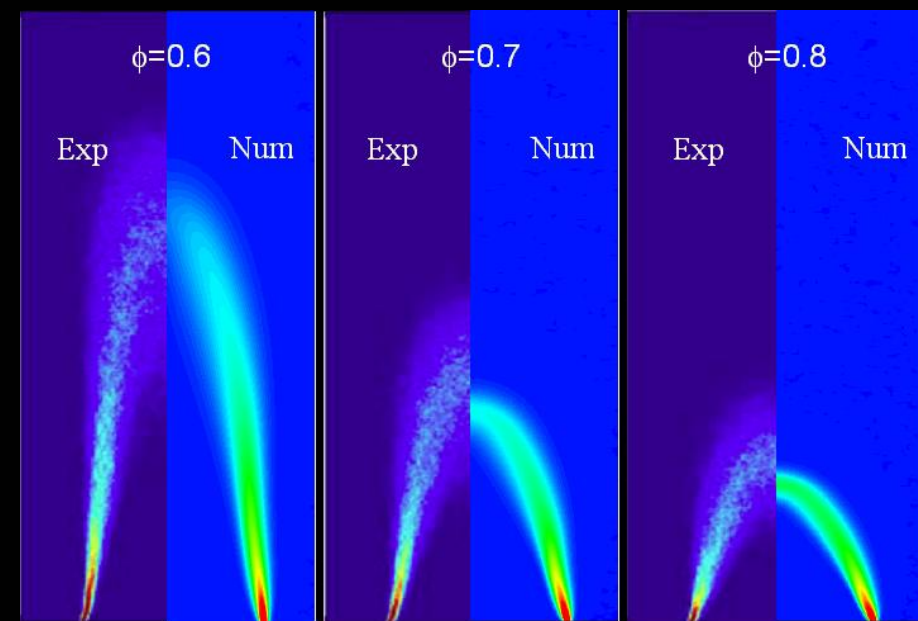
H₂-doped levels – 0, 10, 20 vol %
(with global ϕ constant)

Burner radius, 12.5 mm



HC Premixed Turbulent Flames – Halter et al.

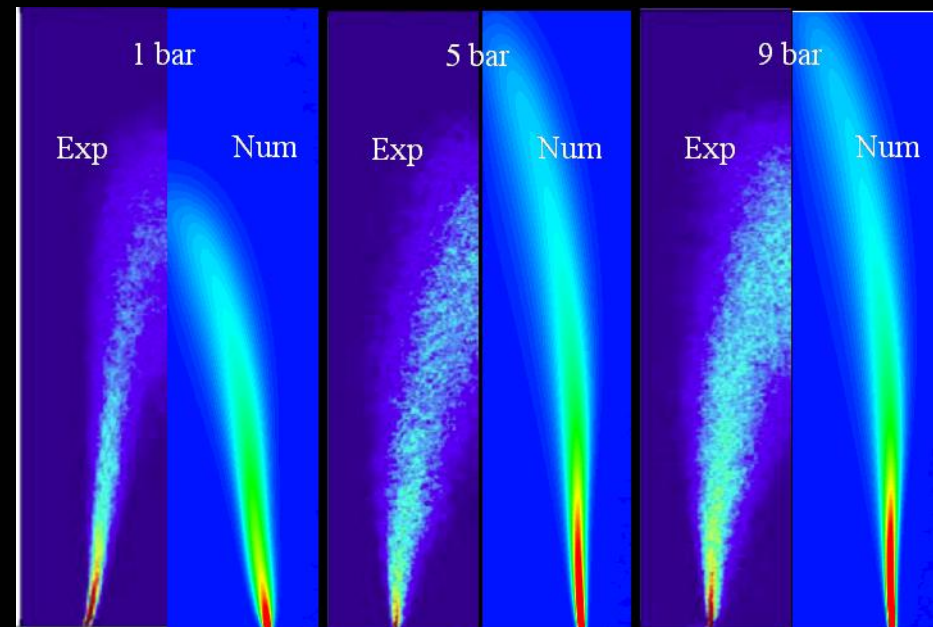
Recent Numerical Simulations vs. Experimental data



Gradient of combustion progress variable

Variation of equivalence ratio →

Pure methane-air mixtures at 1 bar



Gradient of combustion progress variable

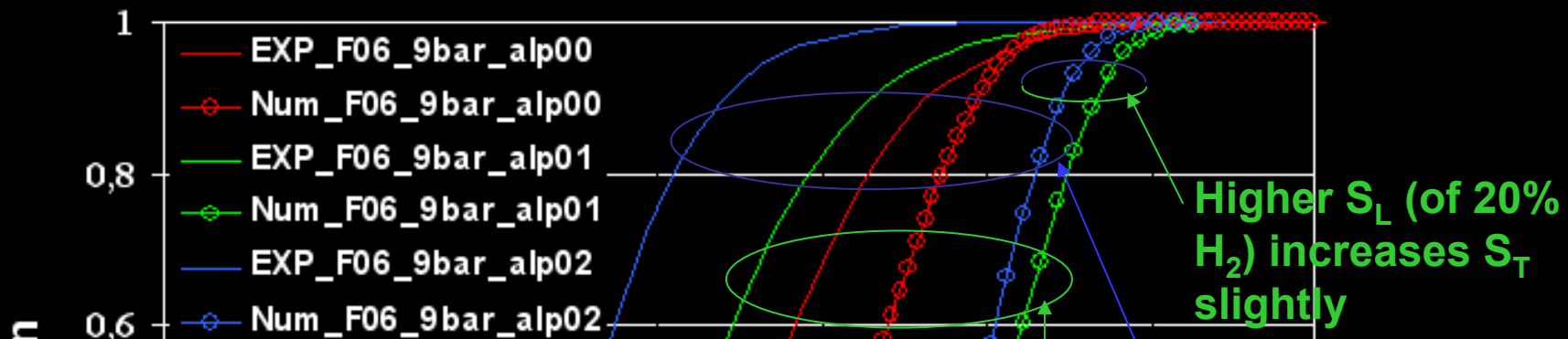
Variation of Pressure →

Pure methane-air mixtures for $\phi=0.6$

Comb. Fl. (in preparation)

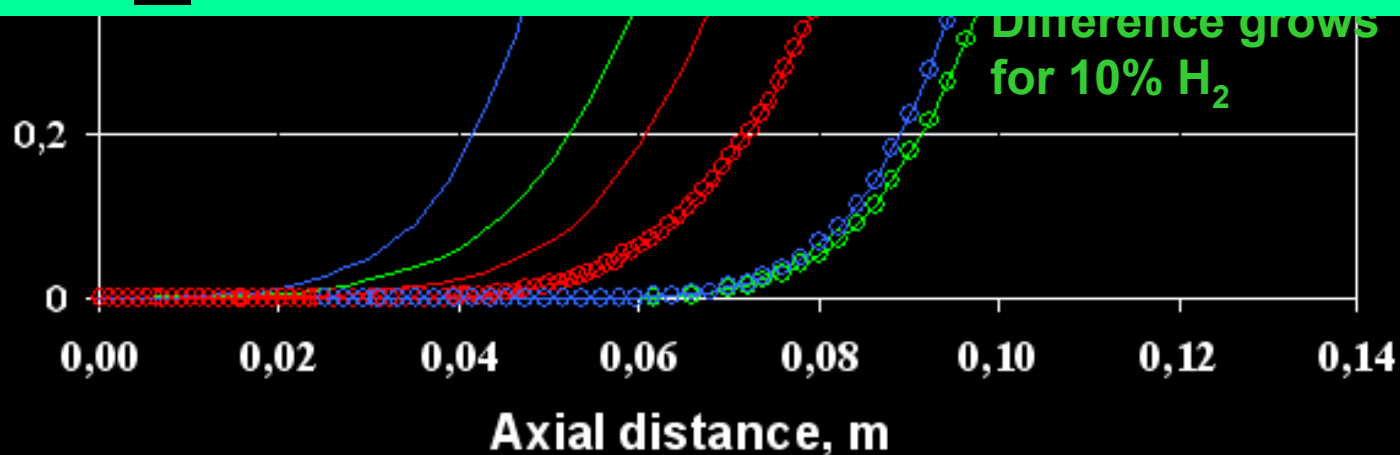
HC & H₂-doped Premixed Turbulent Flames – Halter et al.

Recent Numerical Simulations vs. Experimental data



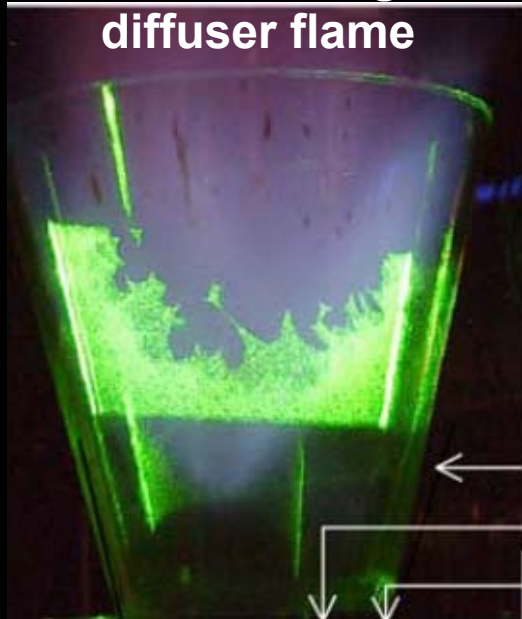
Experiment: 20% H₂ doping increases S_T by 22% - not captured by model

Effective Le does not contribute to this increase



HC & H₂-doped Premixed Turbulent Flames Lawn & Schefer

Novel wide-angled
diffuser flame



Studied flames - 15
(6 pure CH₄ mixtures)

Mixed (CH₄:H₂ - 3:1)

$1 \leq u'/S_{L0} \leq 6$

$U = 2.0 \text{ \& } 3.0 \text{ m/s}$

Measured
Turbulent Displacement Speed

compared with

Model's
Turbulent Flame speed

Bradley's relation

$$S_T = 0.88 \cdot u' \cdot (KaLe)^{-0.3}$$

with

$$Ka = 0.157 \left(\frac{u'}{S_{L0}} \right)^2 Re_t^{-0.5}$$

Present relation

$$S_T = S_L \left(1 + \frac{A}{\exp(Le - 1)} Re_t^{0.25} \left(\frac{u'}{S_L} \right)^{0.3} \right)$$

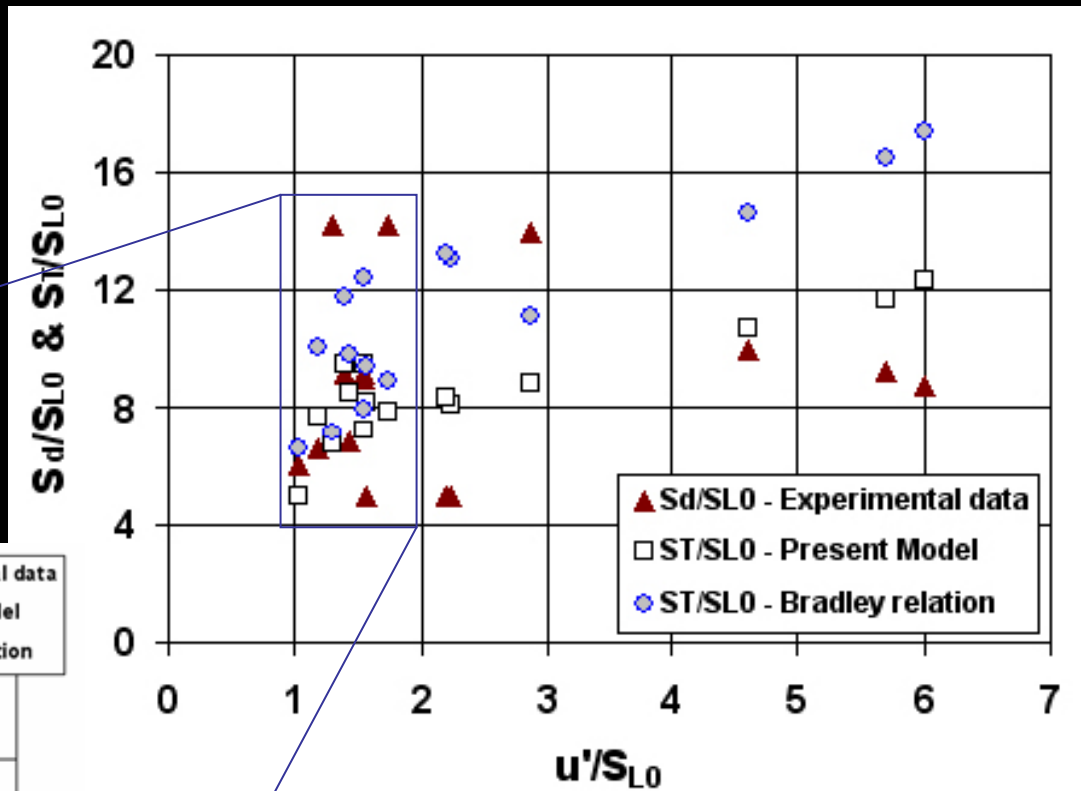
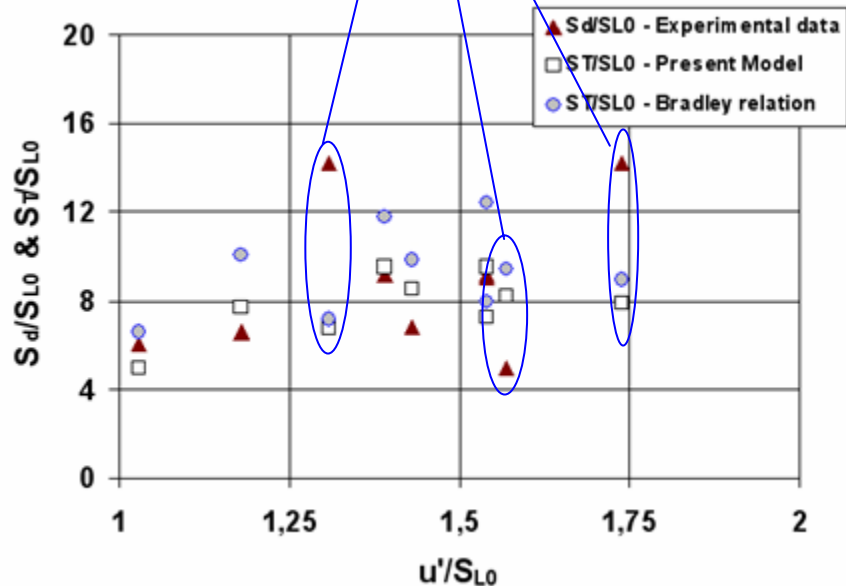
For this data

$$S_L/S_{L0} = (1 - KaMa) \sim 1.0$$

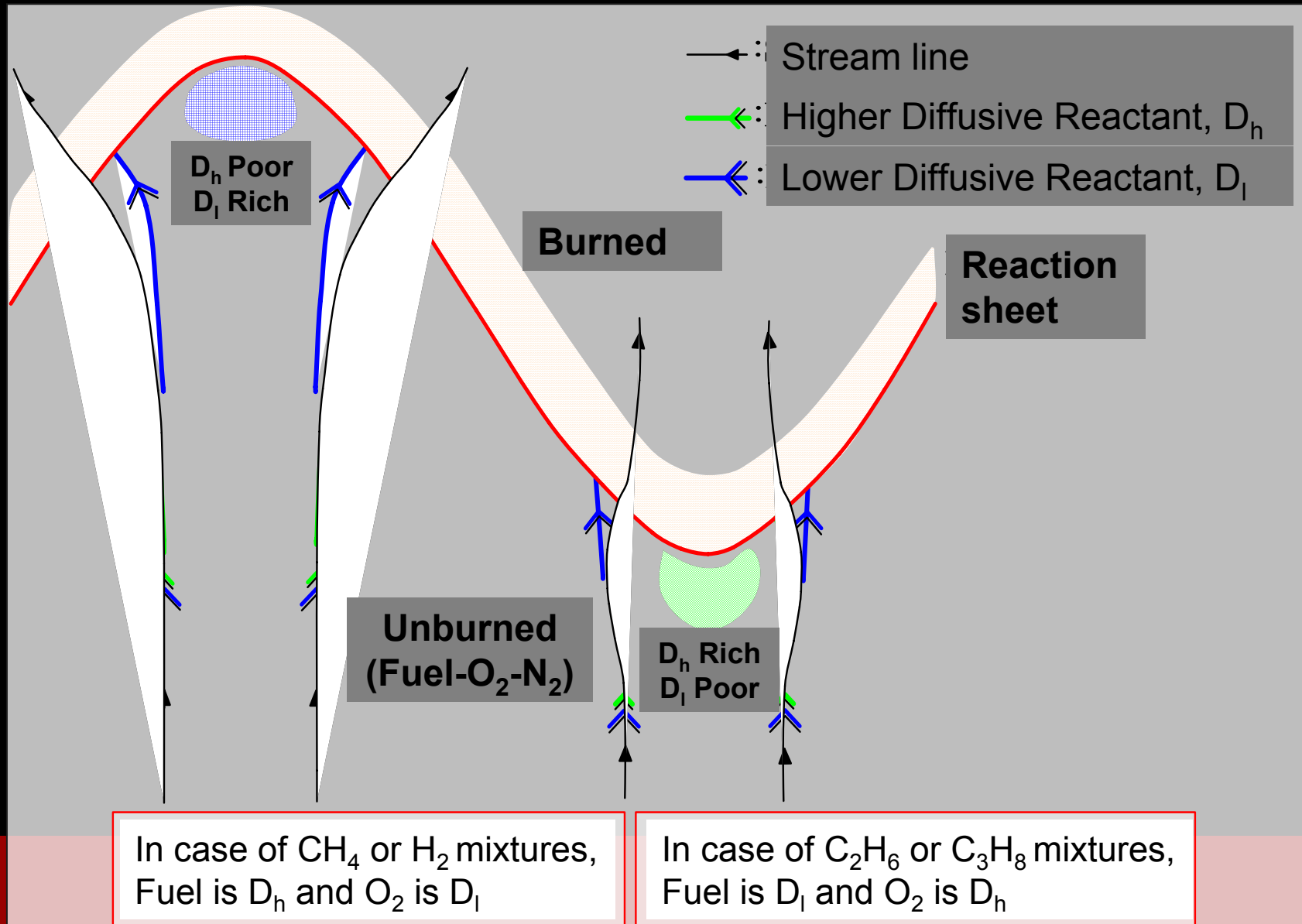
Ma from Halter et al. Comb. Sym. 05

HC & H₂-doped Premixed Turbulent Flames Lawn & Schefer

Difference due to lack of PD effects in the models



Preferential Diffusion Effect



A submodel for Chemical Time Scale

- ✦ Both Le and PD effects can be incorporated into the S_T closure based on the **concept of leading points** — propagation of premixed turbulent flame is controlled by the leading flamelets advancing farthest into the unburned gas
- ✦ In other words, "out of several local reacting structures, those with the highest instantaneous speed rush along other structures and control the turbulent flame speed, which is a strong function of physicochemical characteristics of such leading flamelets via the (critical) chemical time scale τ_{cr} " Lipatnikov and Chomiak

A submodel for Chemical Time Scale

Step 1

$$S_T = S_{L0} + \frac{A}{\exp(Le - 1)} \left(u^{0.8} S_{L0}^{0.2} \right) \left(\frac{\tau_t}{\tau_{c0}} \right)^{1/4} \left(\frac{p}{p_0} \right)^{0.2}$$

$$\tau_{cr} = \tau_{c0} \left(\lim_{t \rightarrow \infty} u_c \right) / \max \{ u_c(t) \}_{r_i = r_{cr}}$$

Critical chemical time scale is deemed to include both PD and Le effects

Step 2

$$A_0 \cdot S_{L0}^{0.2} / \tau_{c0}^{1/4} = A_1 \cdot S_{L1}^{0.2} / \tau_{cr}^{1/4}$$

‡ **A₀ (given), A₁ (unknown)** are model constants

‡ **A₁ estimated from reaction submodel**

‡ **Steps 1 & 2 are analysed for hydrogen influence**

Critical chemical time scale = chemical time scale x consumption rate (of undisturbed planar laminar flame)/maximum possible local consumption rate

Lipatnikov and Chomiak :
Combust. Sym. 1996, CST 1998, PECS 2005

ASME Int. Mech. Congress & Expo 2006

Lipatnikov : Private communication 2006

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Thank you